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Interfacial binding in catalytic and photovoltaic materials, and the energetics of elementary surface processes during catalytic fuels production and utilization[1]

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The fundamental understanding of reactivity trends in organic and inorganic chemistry has led to spectacular scientific advances over the past 50 years in synthetic chemistry. At the basis of this understanding is knowledge of the strengths of the relevant chemical bonds being broken and formed. In this regard, surface chemistry is several decades behind. Yet surface chemical reactivity dictates our choices of materials for energy technology, including catalysts for clean fuels production and utilization, fuel cell electrodes, photocatalysts and photovoltaics. This past decade has seen important advances in our ability to measure surface chemical bond energies and to use them to make predictions of relevance to energy technology. We will review those advances here, with a focus on: (1) the interfacial bonding strength between the metal and the support material in metal nanoparticle catalysts, with emphasis on the roles of particle size and the support in catalyst reactivity and stability, (2) the interfacial reactions that occur between the metal electrode and the semiconducting polymer in organic photovoltaic (OPV) devices, and the heats of those reactions, and (3) the adsorption energies of small molecules on Pt(111), with emphasis on intermediates in catalytic steam reforming, oxidation and dehydrogenation, which reveal a strong correlation between the strength with which adsorbates bond to the Pt(111) surface and their bond energy to the H atom in gas-phase molecules. These measurements provide important benchmarks for comparisons with new computational methods designed to improved energy accuracy beyond standard periodic DFT.

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